

REPORT DOCUMENTATION PAGE

AFRL-SR-AR-TR-05-

The public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing the burden, to Department of Defense, Washington Headquarters Service, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302. Respondents should be aware that notwithstanding any other notice that may appear hereon, it is not authorized by law to impose a collection of information on persons if it does not display a currently valid OMB control number.

PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.

0453

1. REPORT DATE (DD-MM-YYYY)		2. REPORT TYPE Final Report		3. DATES COVERED (From - To) 01 Jul 2003 - 31 Dec 2004	
4. TITLE AND SUBTITLE Atomistic Mechanisms of Fatigue in Nanocrystalline Metals				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER F49620-03-1-0375	
				5c. PROGRAM ELEMENT NUMBER	
				5d. PROJECT NUMBER	
6. AUTHOR(S) Professor Diana Farkas				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Department of Materials Science and Engineering Virginia Tech Blacksburg VA 24061				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) USAF/AFRL AFOSR 875 N. Randolph Street Arlington VA 22203 NA				10. SPONSOR/MONITOR'S ACRONYM(S) AFOSR	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT Distribution Statement A. Approved for public release; distribution is unlimited.					
13. SUPPLEMENTARY NOTES					
14. ABSTRACT We investigate the mechanisms of fatigue behavior in nano-crystalline metals at the atomic scale using empirical force laws and molecular level simulations. A combination of molecular statics and molecular dynamics was used to deal with the time scale limitations of molecular dynamics. We show that the main atomistic mechanism of fatigue crack propagation in these materials is the formation of nano-voids ahead of the main crack. The results obtained for crack advance as a function of stress intensity amplitude are consistent with experimental studies and a Paris law exponent of about 2.					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			19b. TELEPHONE NUMBER (Include area code)
U	U	U	UU	5	

ATOMISTIC MECHANISMS OF FATIGUE IN NANOCRYSTALLINE METALS.

AFOSR GRANT NUMBER F49620-03-1-0375

20051024 097

Diana Farkas, Michael Willemann and Brian Hyde

Dept. of Materials Science and Engineering, Virginia Tech.,

Blacksburg, VA 24061

Abstract

We investigate the mechanisms of fatigue behavior in nano-crystalline metals at the atomic scale using empirical force laws and molecular level simulations. A combination of molecular statics and molecular dynamics was used to deal with the time scale limitations of molecular dynamics. We show that the main atomistic mechanism of fatigue crack propagation in these materials is the formation of nano-voids ahead of the main crack. The results obtained for crack advance as a function of stress intensity amplitude are consistent with experimental studies and a Paris law exponent of about 2.

Research Objective

Fatigue of metallic materials is an important issue in the general field of mechanical behavior. In particular, nano-crystalline materials are particularly susceptible to fatigue failure [1,2]. This constitutes one of the limitations of this new class of metallic materials and the behavior can be generally attributed to the presence of a large fraction of grain boundary material. The details of fatigue failure mechanisms are not well understood. Theoretical models have been generally limited to the macroscopic and meso-scale and no studies have been performed at the atomistic level, to the best of our knowledge [3-6]. There are two basic reasons why fatigue has not been studied atomistically, relating to length scale and time scale. In the present work, we show that with current computing power, we can approach the experimental fatigue length scale of nm/cycle crack extension. The time scale is more problematic. The detailed mechanism by which plasticity affects crack advance is not precisely known and therefore there is no clear way to predict the effects of the unrealistic high cycle loading rates that are possible using molecular dynamics. This key issue of MD time scale (ns) vs. experimental fatigue time scale (s) is addressed in the present work using a combination of molecular statics and molecular dynamics. The combined results of these two techniques are shown to allow the basic understanding of the essential process of crack advance under cyclic loading. We will concentrate mostly on the behavior of Ni. The interatomic interactions for this material have been developed on the basis of first principles data [7] and tested as part of our previous work [8]. Using these potentials, we have previously studied realistic three dimensional polycrystalline samples of pure Ni under monotonic loading conditions. In this letter we report the first simulations under cyclic loading, performed on a digital sample with a columnar grain structure with random misorientations and a 6 nm grain size. Figure 1 shows the rates of crack advance as a function of stress intensity amplitude obtained from both molecular static and molecular dynamic simulations. These results are shown together with experimental results by Hanlon, Kwon and Suresh [10]. Figure 2 shows tip configurations after 26, and 31 cycles. Both configurations are at maximum loading, for the molecular statics simulations and a stress intensity amplitude of 1.4 MPa \sqrt{m} .

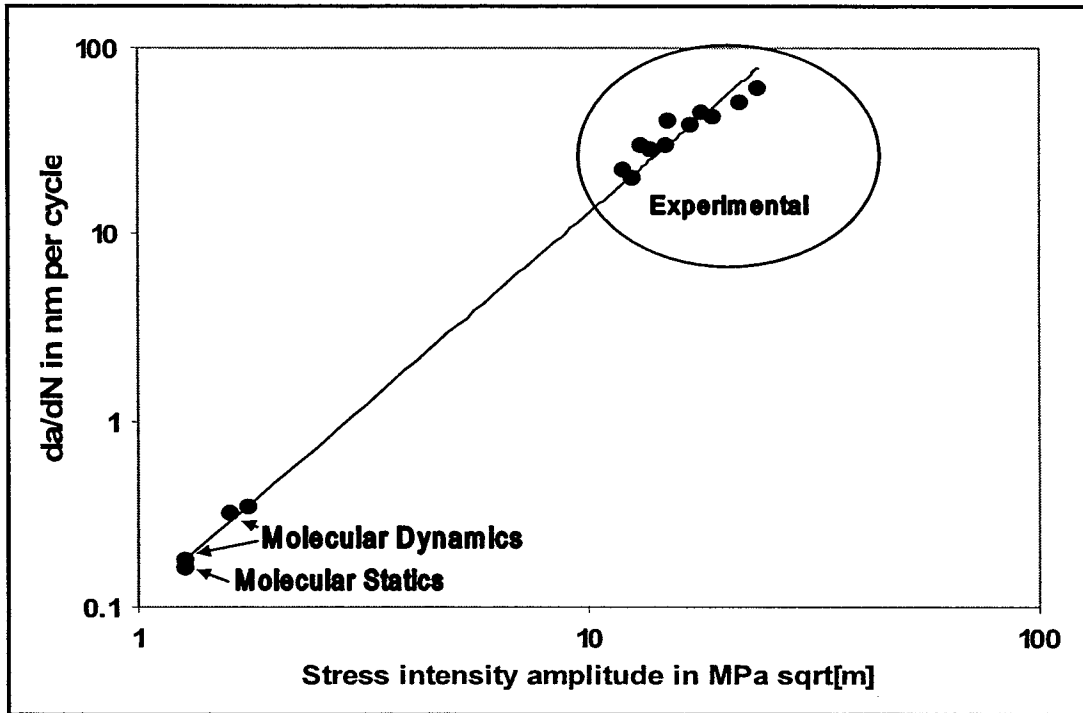


Figure 1: Resulting rate of crack advance for both molecular static and molecular dynamic simulations together with experimental results by Hanlon, Kwon and Suresh [10]

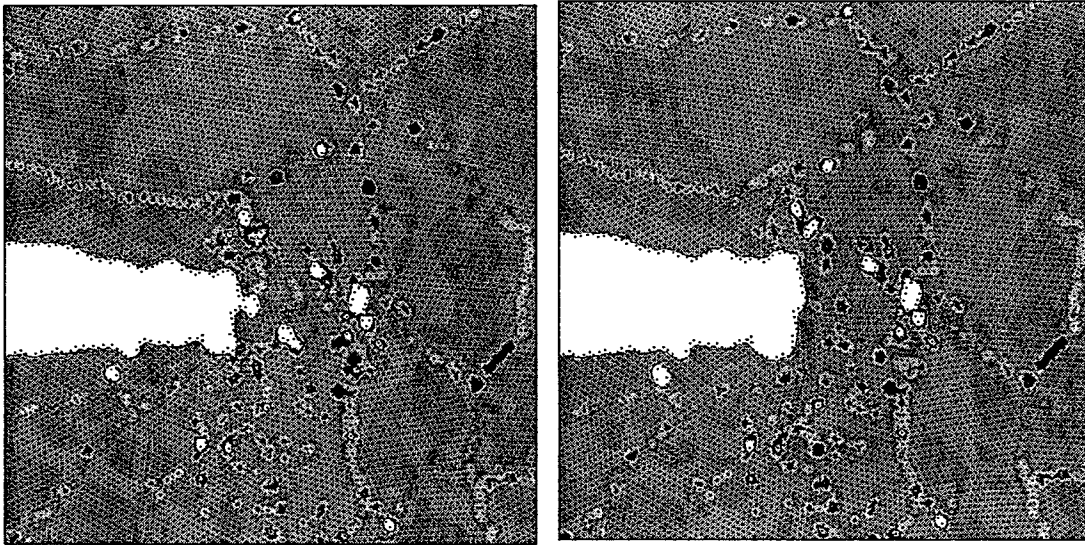


Figure 2: tip configurations after 26, and 31 cycles. Each picture is taken at maximum loading, for the simulations conducted using molecular statics and a stress intensity amplitude of 1.4 MPa \sqrt{m} .

Acknowledgment/Disclaimer

This work was sponsored by the Air Force Office of Scientific Research, USAF, under grant/contract number F49620-03-1-0375. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the Air Force Office of Scientific Research or the U.S. Government.

References

1. Kumar, KS; Van Swygenhoven, H; Suresh, S, Mechanical behavior of nanocrystalline metals and alloys, ACTA MATER, 51 (19): 5743-5774 NOV 25, 2003.
2. Weertman, JR; Farkas, D; Hemker, K; et al. , Structure and mechanical behavior of bulk nanocrystalline materials, MRS BULL, 24 (2): 44-50 FEB, 1999.
3. Deshpande, VS; Needleman, A; Van der Giessen, E, Scaling of discrete dislocation predictions for near-threshold fatigue crack growth, ACTA MATER, 51 (15): 4637-4651 SEP 3, 2003
4. Deshpande, VS; Needleman, A; Van der Giessen, E Discrete dislocation plasticity modeling of short cracks in single crystals, ACTA MATER, 51 (1): 1-15 JAN 8, 2003.
5. Deshpande, VS; Needleman, A; Van der Giessen, E, Discrete dislocation modeling of fatigue crack propagation, ACTA MATER, 50 (4): 831-846 FEB 25, 2002.
6. Deshpande, VS; Needleman, A; Van der Giessen, E , A discrete dislocation analysis of near-threshold fatigue crack growth, ACTA MATER, 49 (16): 3189-3203 SEP 20, 2001.
7. Mishin, Y; Farkas, D; Mehl, MJ; et al., Interatomic potentials for monoatomic metals from experimental data and ab initio calculations, PHYS REV B, 59 (5): 3393-3407 FEB 1 1999.
8. Farkas, D; Van Swygenhoven, H; Derlet, PM, Intergranular fracture in nanocrystalline metals, PHYS REV B, 66 (6): art. no.-060101 AUG 1, 2002
9. Van Swygenhoven, H; Spaczer, M; Caro, A; et al., Competing plastic deformation mechanisms in nanophase metals, PHYS REV B, 60 (1): 22-25 JUL 1 , 1999.
10. Hanlon, T; Kwon, YN; Suresh, S, Grain size effects on the fatigue response of nanocrystalline metals, SCRIPTA MATER, 49 (7): 675-680 OCT 2003.

Personnel Supported

Mike Willemann	Undergraduate Student, Virginia Tech.
Brian Hyde	Graduate Student, Virginia Tech
Diana Farkas	Professor, Virginia Tech.

Publications

"ATOMISTIC MECHANISMS OF FATIGUE IN NANOCRYSTALLINE METALS" D. Farkas, Mike Willemann and B. Hyde" to be submitted

Awards Received

Diana Farkas, Alumni Research Award, Virginia Tech, Fall 2003.